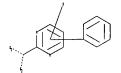
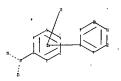
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Uploading C:\Program Files\Stnexp\Queries\10564013.str





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chain nodes :
17 19 21
ring nodes :
1 2 3 4 5 6 7 8 9 10 11 12
ring/chain nodes :
chain bonds :
3-17 17-19 17-21
ring bonds :
                  4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
1-2 1-6 2-3 3-4
exact/norm bonds :
17-19 17-21
exact bonds :
3-17
normalized bonds :
1-2 1-6 2-3 3-4 4-5 5-6 7-8 7-12 8-9 9-10 10-11 11-12
isolated ring systems :
containing 7 :
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G1:0,Cl,Br,F,I

G2:0, N

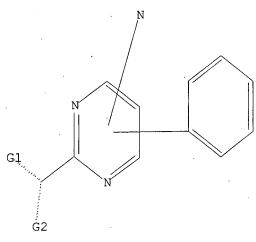
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1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom
11:Atom 12:Atom 13:CLASS 15:Atom 16:Atom 17:CLASS 19:CLASS 21:CLASS

L1 STRUCTURE UPLOADED

=> d 11

L1 HAS NO ANSWERS

L1 STR



G1 O,Cl,Br,F,I

G2 O, N

Structure attributes must be viewed using STN Express query preparation.

=> s 11 sss sam

SAMPLE SEARCH INITIATED 23:02:38 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED - 1415 TO ITERATE

100.0% PROCESSED 1415 ITERATIONS

3 ANSWERS

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

.PROJECTED ITERATIONS: 26044 TO 30556

PROJECTED ANSWERS: 3 TO 163

L2 3 SEA SSS SAM L1

=> => s 11 sss ful FULL SEARCH INITIATED 23:03:31 FILE 'REGISTRY' FULL SCREEN SEARCH COMPLETED - 29728 TO ITERATE

100.0% PROCESSED 29728 ITERATIONS 69 ANSWERS SEARCH TIME: 00.00.01

.

L3 69 SEA SSS FUL L1

=> => s 13 L4 8 L3

=> d 14 1-8 bib, ab, hitstr

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L4
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ΑN
     2007:354856 CAPLUS
DN
     146:380000
ΤI
     Preparation of substituted 2-hydroxylaminopyrimidines as agricultural
     fungicides
     Rheinheimer, Joachim; Grote, Thomas; Mueller, Bernd; Lohmann, Jan Klaas;
ΙN
     Grammenos, Wassilios; Huenger, Udo; Schieweck, Frank; Ulmschneider, Sarah;
     Dietz, Jochen; Renner, Jens; Speakman, John-Bryan; Scherer, Maria;
     Strathmann, Siegfried; Stierl, Reinhard
PΑ
     BASF A.-G., Germany
SO
     Ger. Offen., 89pp.
                                                       Common For
     CODEN: GWXXBX
DT
     Patent
LA
     German
FAN.CNT 1
                                 DATE
     PATENT NO.
                         KIND
                                             APPLICATION NO.
                                                                     DATE
                                             -----
                                 20070329
     DE 102005046592
                                             DE 2005-102005046592
PI.
                          Α1
                                                                     20050928
                                 20070405
     WO 2007036477
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                                             WO 2006-EP66572
                                                                     20060921
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             RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ,
             UA, UG, US, UZ, VC, VN, ZA, ZM, ZW
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             CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
             GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
                                                      no pending US apple.
             KG, KZ, MD, RU, TJ, TM
PRAI DE 2005-102005046592 A
                                 20050928
OS
     MARPAT 146:380000
AΒ
     Title compds. [I; R1, R2 = H, (halo)alkyl, (halo)alkenyl, (halo)alkynyl,
     (halo)cycloalkyl, etc. or R1NOR2 = 5-7 membered (saturated) (substituted)
     heterocyclyl; R3 = halo, cyano, azido, (substituted) (halo)alkyl,
     (halo)alkenyl, (halo)alkynyl, etc.; R4 = 5-6 membered (saturated) aromatic
     (substituted) heterocyclyl containing O, N and S; B = Ph, 5-6 membered
     heteroaryl containing O, N and S; L = halo, cyano, OCN, (halo)alkyl,
     (halo)alkenyl, (halo)alkynyl, etc.; n = 1-5], were prepared Thus, 95% NaH
     in THF was stirred with 1,2,4-triazole for 3 h at room temperature followed by
     stirring with 4-chloro-2-methylsulfonyl-6-(6-methyltetrahydro-2H-1,2-
     oxazin-2-yl)-5-(2,4,6-trifluorophenyl)pyrimidine (preparation given) over night
     at room temperature to give
4-chloro-6-(6-methyltetrahydro-2H-1,2-oxazin-2-yl)-2-
     (1,2,4-\text{triazol}-1-\text{yl})-5-(2,4,6-\text{trifluorophenyl}) pyrimidine.
                                                                  The latter as a
     250 ppm spray on tomato leaves infected with Alternaria solani reduced the
     infection to 20%, vs. 90% for untreated controls.
     931118-01-3P 931118-17-1P 931118-20-6P
ΙT
     931118-31-9P
     RL: AGR (Agricultural use); BSU (Biological study, unclassified); SPN
     (Synthetic preparation); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (preparation of substituted hydroxylaminopyrimidines as agricultural
        fungicides)
RN
     931118-01-3 CAPLUS
     2-Pyrimidinecarboxamide, 4-chloro-6-(2-isoxazolidinyl)-5-(2,4,6-
CN
```

trifluorophenyl) - (CA INDEX NAME)

$$\begin{array}{c|c} O & & \\ H_2N-C & N & Cl & F \\ \hline N & & & F \\ \hline \end{array}$$

RN 931118-17-1 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2-chloro-4-fluorophenyl)-6-(methoxymethylamino)- (CA INDEX NAME)

$$\begin{array}{c|c} O & \\ \parallel \\ H_2N-C & N & R \\ \hline N & \\ C1 & C1 \end{array}$$

RN 931118-20-6 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2-chloro-4-fluorophenyl)-6-[methyl(1-methylethoxy)amino]- (CA INDEX NAME)

$$\begin{array}{c|c} O & & \\ H_2N-C & N & R \\ \hline & N & \\ & C1 & C1 \end{array}$$

RN 931118-31-9 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-6-(tetrahydro-2H-1,2-oxazin-2-yl)-5-(2,4,6-trifluorophenyl)- (CA INDEX NAME)

$$H_2N-C$$
 N
 $C1$
 F
 F

```
L4
      ANSWER 2 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
AN
      2006:768723 CAPLUS
DN
      145:180954
TΙ
      Substituted 5-phenylpyrimidines for use in cancer therapy
IN
      Rheinheimer, Joachim; Grote, Thomas; Mueller, Bernd; Nave, Barbara;
      Schieweck, Frank; Schwoegler, Anja; Jabs, Thorsten; Blettner, Carsten
PA
      BASF Aktiengesellschaft, Germany
SO
      PCT Int. Appl., 60pp.
                                                                       Lower Du
      CODEN: PIXXD2
DT
      Patent
LA
      English
FAN.CNT 1
                              KIND
                                      DATE
      PATENT NO.
                                                    APPLICATION NO.
                              ____
                               Α2
                                      20060803
                                                    WO 2006-EP774
PΙ
      WO 2006079556
                                                                                20060130
      WO 2006079556
                              А3
                                      2006092
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               CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
               GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX,
               MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC,
               VN, YU, ZA, ZM, ZW
          RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
               KG, KZ, MD, RU, TJ, TM
                                                      no pending US apple
PRAI EP 2005-1955
                                      20050131
                               Α
OS
      MARPAT 145:180954
AΒ
      The invention discloses substituted 5-phenylpyrimidines I [X = NR1R2,
      OR1a, SR1a, (R1, R2 = H, C1-C10 alkyl, C2-C6-alkenyl, etc.; R1a = R1
      except for hydrogen); Y = halo, cyano, C1-C4-alkyl, etc.; R4 = radical of
      1-15 atoms different from H; L = radical of 1-10 atoms different from H; n
      = 0-5], or a pharmaceutically acceptable salt thereof, for use in therapy,
      in particular for the therapy of cancerous diseases.
ΙT
      838838-62-3 838838-71-4 838838-82-7
      838838-84-9 838838-88-3 838838-89-4
      903549-09-7 903549-10-0 903549-20-2
      903549-35-9
      RL: PAC (Pharmacological activity); THU (Therapeutic use); BIOL
      (Biological study); USES (Uses)
          (phenylpyrimidine derivs. for cancer therapy)
RN
      838838-62-3 CAPLUS
CN
      2-Pyrimidinecarboxamide, 4-chloro-6-[[(1S)-2,2,2-trifluoro-1-
     methylethyl]amino]-5-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)
```

RN 838838-71-4 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-N-methyl-6-[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 838838-82-7 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2,6-difluorophenyl)-6-(4-methyl-1-piperidinyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & \text{C1} \\ & \text{F} \\ & \text{N} \\ & \text{N} \\ & \text{O} \\ & \text{Me} \\ \end{array}$$

RN 838838-84-9 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2,6-difluorophenyl)-6-[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]- (9CI) (CA INDEX NAME)

RN 838838-88-3 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2-chloro-4-methoxyphenyl)-6-[[(1S)-1,2-dimethylpropyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 838838-89-4 CAPLUS

CN 2-Pyrimidinecarboxamide, N-acetyl-4-chloro-5-(2,6-difluorophenyl)-6-(4-methyl-1-piperidinyl)- (9CI) (CA INDEX NAME)

RN 903549-09-7 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2,6-difluoro-4-methoxyphenyl)-6-(4-methyl-1-piperidinyl)- (9CI) (CA INDEX NAME)

RN 903549-10-0 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2,6-difluoro-4-methoxyphenyl)-6-[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 903549-20-2 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2,6-difluoro-4-methoxyphenyl)-6-[[(1S)-1,2-dimethylpropyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 903549-35-9 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2-chloro-4-methoxyphenyl)-6-[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]- (9CI) (CA INDEX NAME)

```
ANSWER 3 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
L4
     2005:120896 CAPLUS
AN
DN
     142:198096
ΤI
     Preparation of 2-acyl-4-amino-5-arylpyrimidines as pesticides and
     fungicides.
IN
     Schwoeqler, Anja; Gewehr, Markus; Mueller, Bernd; Grote, Thomas;
     Grammenos, Wassilios; Tormo I. Blasco, Jordi; Gypser, Andreas;
     Rheinheimer, Joachim; Blettner, Carsten; Schaefer, Peter; Schieweck,
     Frank; Wagner, Oliver; Stierl, Reinhard; Schoefl, Ulrich; Strathmann,
     Siegfried; Scherer, Maria
PA
     BASF Aktiengesellschaft, Germany
SO
     PCT Int. Appl., 79 pp.
     CODEN: PIXXD2
DT
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LA
     German
FAN.CNT 2
     PATENT NO.
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                                                WO 2004-EP7877
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              LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
              NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
              TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
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              AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK,
              EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE,
              SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE,
              SN, TD, TG
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                                   20060503
                                                EP 2004-741053
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                                   20070103
                            B1
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                                   20061003
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                            T
                                   20061221
                                                JP 2006-520743
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                                   20070115
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                                   20060321
                                                MX 2006-PA38
                                                                         20060105
     IN 2006CN00644
                            Α
                                   20070608
                                                IN 2006-CN644
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                            Α1
                                   20070510
                                                US 2007-564013
                                                                         20070109
PRAI DE 2003-10333857
                            Α
                                   20030724
     DE 2003-10357714
                            Α
                                   20031209
     WO 2004-EP7877
                            W
                                   20040715
OS
     MARPAT 142:198096
AB
     Title compds. [I; n = 1-5; L = halo, cyano, cyanato, alkyl, alkenyl,
     alkynyl, alkoxy, alkenyloxy, alkynyloxy, cycloalkyl, cycloalkoxy, etc.;
     R1, R2 = (substituted) alkyl, alkenyl, alkynyl, cycloalkyl,
     halocycloalkyl; R1R2N = atoms to form 5-6 membered (substituted)
     heterocyclyl; R3 = halo, cyano, alkyl, alkenyl, alkynyl, cycloalkyl,
     alkoxy, alkenyloxy, alkynyloxy, alkylthio, etc.; R4 = CONHXRa, C(ORb):NXRa; X = bond, CO, CONH, CO2, O, imino, etc.; Ra = H, alkyl, alkenyl, alkynyl, PhCH2; Rb = H, alkyl, alkenyl, alkynyl], were prepared
     Thus, (S)-4-chloro-6-(2,2,2-trifluoro-1-methylethylamino)-5-(2,4,6-
     trifluorophenyl)pyrimidine-2-carbonitrile was stirred with K2CO3 and H2O2
     in Me2SO at 10°-room temperature to give (S)-4-chloro-6-(2,2,2-trifluoro-
     1-methylethylamino)-5-(2,4,6-trifluorophenyl)pyrimidine-2-carboxamide.
```

The latter at 250 ppm on tomatoes gave complete protection against

```
Phytophthora infestans.
ΙT
     838838-58-7P 838838-59-8P 838838-60-1P
     838838-61-2P 838838-62-3P 838838-63-4P
     838838-64-5P 838838-65-6P 838838-66-7P
     838838-67-8P 838838-68-9P 838838-69-0P
     838838-70-3P 838838-71-4P 838838-72-5P
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     838838-97-4P 838838-98-5P 838838-99-6P
     838839-00-2P 838839-01-3P 838839-02-4P
     838839-03-5P 838839-04-6P 838839-05-7P
     838839-06-8P 838839-07-9P 838839-08-0P
     838839-09-1P 838839-10-4P 838839-11-5P
     838839-12-6P
     RL: AGR (Agricultural use); BSU (Biological study, unclassified); BUU
     (Biological use, unclassified); SPN (Synthetic preparation); BIOL
     (Biological study); PREP (Preparation); USES (Uses)
        (preparation of acylaminoarylpyrimidines as pesticides and fungicides)
RN
     838838-58-7
                 CAPLUS
CN
     2-Pyrimidinecarboxamide, 4-chloro-6-[(1,2-dimethylpropyl)amino]-5-(2,4,6-
     trifluorophenyl) - (9CI)
                              (CA INDEX NAME)
```

RN 838838-59-8 CAPLUS
CN 2-Pyrimidinecarboxamide, 4-chloro-6-(4-methyl-1-piperidinyl)-5-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)

RN 838838-60-1 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2-chloro-6-fluorophenyl)-6-[(1-methylethyl)amino]- (9CI) (CA INDEX NAME)

RN 838838-61-2 CAPLUS

CN 2-Pyrimidinecarboxylic acid, 4-chloro-5-(2-chloro-6-fluorophenyl)-6-[(1-methylethyl)amino]-, hydrazide (9CI) (CA INDEX NAME)

RN 838838-62-3 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-6-[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)

RN 838838-63-4 CAPLUS

CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)-, hydrazide (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 838838-64-5 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-6-(di-2-propenylamino)-5-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)

RN 838838-65-6 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-6-(di-2-propenylamino)-N-methyl-5-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & \text{CH}_2\text{--}\text{CH} \Longrightarrow \text{CH}_2 \\ & & \text{N--}\text{CH}_2\text{--}\text{CH} \Longrightarrow \text{CH}_2 \\ & & \text{N--}\text{CH}_2\text{--}\text{CH} \Longrightarrow \text{CH}_2 \\ & & & \text{F} \end{array}$$

RN 838838-66-7 CAPLUS

CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)-, 2,2-dimethylhydrazide (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 838838-67-8 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-N-(1,1-dimethylethyl)-6-[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 838838-68-9 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-N-hydroxy-6-[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 838838-69-0 CAPLUS

CN 2-Pyrimidinecarboxamide, N-acetyl-4-chloro-6-[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 838838-70-3 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-6-[(2,2,2-trifluoro-1-methylethyl)amino]-5-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)

RN 838838-71-4 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-N-methyl-6-[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)

RN 838838-72-5 CAPLUS

CN Glycine, N-[2-(aminocarbonyl)-6-chloro-5-(2,4,6-trifluorophenyl)-4-pyrimidinyl]- (9CI) (CA INDEX NAME)

$$H_2N-C$$
 N
 $NH-CH_2-CO_2H$
 F
 F

RN 838838-73-6 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-6-[[(1R)-1,2-dimethylpropyl]amino]-5-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 838838-74-7 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2-chloro-4-fluorophenyl)-6-[(1-methylethyl)amino]- (9CI) (CA INDEX NAME)

RN 838838-75-8 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2-chloro-4-fluorophenyl)-6-[(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

RN 838838-76-9 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2,4-difluorophenyl)-6-[[(1R)-1,2-dimethylpropyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 838838-77-0 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2,4-difluorophenyl)-6-[(phenylmethyl)amino]- (9CI) (CA INDEX NAME)

$$H_2N-C$$
 N
 $NH-CH_2-Ph$
 N
 F

RN 838838-78-1 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2,4-difluorophenyl)-6-[(1-methylethyl)amino]- (9CI) (CA INDEX NAME)

RN 838838-79-2 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2,4-difluorophenyl)-6-(4-methyl-1-piperidinyl)- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} F & C1 \\ \hline N & C-NH_2 \\ \hline Me & O \end{array}$$

RN 838838-80-5 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2,4-difluorophenyl)-6-[[(1S)-1,2-dimethylpropyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 838838-81-6 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2-chloro-4-fluorophenyl)-6-[[(1S)-1,2-dimethylpropyl]amino]- (9CI) (CA INDEX NAME)

RN 838838-82-7 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2,6-difluorophenyl)-6-(4-methyl-1-piperidinyl)- (9CI) (CA INDEX NAME)

RN 838838-83-8 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2-chloro-4-fluorophenyl)-6-(4-methyl-1-piperidinyl)- (9CI) (CA INDEX NAME)

RN 838838-84-9 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2,6-difluorophenyl)-6-[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]- (9CI) (CA INDEX NAME)

RN 838838-85-0 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2,6-difluorophenyl)-6-[[(1S)-1,2-dimethylpropyl]amino]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 838838-86-1 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2-chloro-4-fluorophenyl)-6-[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 838838-87-2 CAPLUS

CN 2-Pyrimidinecarboxamide, N-acetyl-4-chloro-5-(2-chloro-4-fluorophenyl)-6-(4-methyl-1-piperidinyl)- (9CI) (CA INDEX NAME)

RN 838838-88-3 CAPLUS

CN 2-Pyrimidinecarboxamide, 4-chloro-5-(2-chloro-4-methoxyphenyl)-6-[[(1S)-1,2-dimethylpropyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 838838-89-4 CAPLUS

CN 2-Pyrimidinecarboxamide, N-acetyl-4-chloro-5-(2,6-difluorophenyl)-6-(4-methyl-1-piperidinyl)- (9CI) (CA INDEX NAME)

RN 838838-90-7 CAPLUS

CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)-, methyl ester (9CI) (CA INDEX NAME)

RN 838838-91-8 CAPLUS

CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-(di-2-propenylamino)-5-(2,4,6-trifluorophenyl)-, 1-methylethyl ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & CH_2-CH \Longrightarrow CH_2 \\ i-PrO-C & N-CH_2-CH \Longrightarrow CH_2 \\\hline \\ N & F \end{array}$$

RN 838838-92-9 CAPLUS

CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)-, 1-methylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 838838-93-0 CAPLUS

CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)-, ethyl ester (9CI) (CA INDEX NAME)

RN 838838-94-1 CAPLUS

CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)-, propyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 838838-95-2 CAPLUS

CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[(2,2,2-trifluoroethyl)amino]-5-(2,4,6-trifluorophenyl)-, 1-methylethyl ester (9CI) (CA INDEX NAME)

RN 838838-96-3 CAPLUS

CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)-, butyl ester (9CI) (CA INDEX NAME)

RN 838838-97-4 CAPLUS

CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)-, pentyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Me
$$S$$
 CF3

Me S CF3

N NH

F

RN 838838-98-5 CAPLUS

CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)-, hexyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 838838-99-6 CAPLUS

CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)-, 2,2,2-trifluoroethyl ester (9CI) (CA INDEX NAME)

RN 838839-00-2 CAPLUS

CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)-, 3-methylbutyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 838839-01-3 CAPLUS

CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)-, 2-methylbutyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 838839-02-4 CAPLUS

CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)-, 1-methylbutyl ester (9CI) (CA INDEX NAME)

RN 838839-03-5 CAPLUS

CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-(4-methyl-1-piperidinyl)-5-(2,4,6-trifluorophenyl)-, 1-methylethyl ester (9CI) (CA INDEX NAME)

RN 838839-04-6 CAPLUS

CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)-, 1,2-dimethylpropyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 838839-05-7 CAPLUS

CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)-, 2-propenyl ester (9CI) (CFINDEX NAME)

RN 838839-06-8 CAPLUS

CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)-, 2-aminoethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 838839-07-9 CAPLUS

CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)-, cyclohexyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 838839-08-0 CAPLUS

CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)-, 2-methylpropyl ester (9CI)

(CA INDEX NAME)

Absolute stereochemistry.

RN 838839-09-1 CAPLUS

CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)-, 1-methylpropyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 838839-10-4 CAPLUS

CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 838839-11-5 CAPLUS

CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)-, cyclopentyl ester (9CI)

(CA INDEX NAME)

Absolute stereochemistry.

RN 838839-12-6 CAPLUS

CN 2-Pyrimidinecarboxylic acid, 4-chloro-6-[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)-, cyclobutyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 838839-13-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of acylaminoarylpyrimidines as pesticides and fungicides)

RN 838839-13-7 CAPLUS

CN 2-Pyrimidinecarbonyl chloride, 4-chloro-6-[[(1S)-2,2,2-trifluoro-1-methylethyl]amino]-5-(2,4,6-trifluorophenyl)- (9CI) (CA INDEX NAME)

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L4
     ANSWER 4 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
ΑN
     2004:817651
                 CAPLUS
DN
     141:332206
     Preparation of biaryl substituted 6-membered heterocycles as sodium channel blockers
ΤI
ΙN
     Chakravarty, Prasun K.; Fisher, Michael H.; Parsons, William H.; Liang,
     Jun; Zhou, Bishan
PA
     Merck & Co., Inc., USA
SO
     PCT Int. Appl., 125 pp.
     CODEN: PIXXD2
DT
     Patent
LA
     English
FAN.CNT 1
     PATENT NO.
                         KIND
                                DATE
                                             APPLICATION NO.
                                                                    DATE
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     _____
                                            WO 2004-US8532
PΙ
     WO 2004084824
                          Α2
                                20041007
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                                20050331
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             CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD,
             GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC,
             LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI,
             NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY,
             TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
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     AU 2004224392
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                                                                    20040319
     CA 2519677
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    EP 1608622
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             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK
                                20060621
                                                                    20040319
     CN 1791580
                                             CN 2004-80013599
                          Α
     JP 2006521357
                          Т
                                20060921
                                             JP 2006-507395
                                                                    20040319
     US 2006293339
                                             US 2005-550641
                          Α1
                                20061228
                                                                    20050923
PRAI US 2003-456312P
                          Ρ
                                20030324
     WO 2004-US8532
                                20040319
                          Α
OS
     MARPAT 141:332206
AB
     The title biaryl substituted pyridine, pyrimidine and pyrazine compds. [I
     or II; H-1 = (un) substituted pyridyl, pyrimidyl, pyrazinyl; H-2 =
     (un) substituted pyridyl, pyrimidyl, pyrazinyl; R4, R5 = H, alkyl, alkoxy,
     aryloxy, etc.; R6-R8 = H, alkyl, cycloalkyl, alkoxy, etc.] which are
     sodium channel blockers useful for the treatment of pain (no data), were
     prepared E.g., a 2-step synthesis of III, starting from
     2-bromo-6-methylpyridine and 3-bromophenylboronic acid, was given.
     Claimed pharmaceutical compns. comprise an effective amount of the instant
     compds. I, either alone, or in combination with one or more
     therapeutically active compds., and a pharmaceutically acceptable carrier.
     Methods of treating conditions associated with, or caused by, sodium channel
     activity, including, for example, acute pain, chronic pain, visceral pain,
     inflammatory pain, neuropathic pain, epilepsy, irritable bowel syndrome,
     depression, anxiety, multiple sclerosis, and bipolar disorder, comprise
     administering an effective amount of the present compds., either alone, or
     in combination with one or more other therapeutically active compds.
IT
     770727-12-3P
     RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
     (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
     (Uses)
        (preparation of biaryl substituted 6-membered heterocycles as sodium channel
```

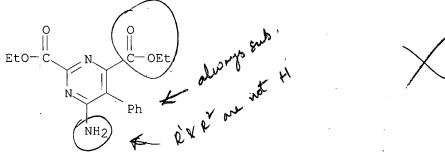
blockers for treatment or prevention of pain) 770727-12-3 CAPLUS

RN CN

2-Pyrimidinecarboxamide, 4-amino-6-[2'-(trifluoromethoxy)[1,1'-biphenyl]-3yl]- (9CI) (CA INDEX NAME)

-NH2

- L4 ANSWER 5 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
- AN 2004:205964 CAPLUS
- DN 142:74474
- TI Product class 12: pyrimidines
- AU von Angerer, S.
- CS Germany
- SO Science of Synthesis (2004), 16, 379-572 CODEN: SSCYJ9
- PB Georg Thieme Verlag
- DT Journal; General Review
- LA English
- AB A review. Methods for preparing pyrimidines are reviewed including cyclization, ring transformation, aromatization and substituent modification.
- IT 157201-09-7P
 - RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of pyrimidines via cyclization, ring transformation, aromatization and substituent modification)
- RN 157201-09-7 CAPLUS
- CN 2,4-Pyrimidinedicarboxylic acid, 6-amino-5-phenyl-, diethyl ester (9CI) (CA INDEX NAME)



RE.CNT 856 THERE ARE 856 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

- L4 ANSWER 6 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
- AN 2003:385500 CAPLUS
- DN 139:111073
- TI QSAR Study of Ethyl $2-[(3-Methyl-2,5-dioxo(3-pyrrolinyl))amino]-4-(trifluoromethyl) pyrimidine-5-carboxylate: An Inhibitor of AP-1 and NF-<math>\kappa$ B Mediated Gene Expression Based on Support Vector Machines
- AU Liu, H. X.; Zhang, R. S.; Yao, X. J.; Liu, M. C.; Hu, Z. D.; Fan, B. T.
- CS Department of Chemistry, Department of Computer Science and State Key Laboratory of Applied Organic Chemistry, Lanzhou University, Lanzhou, 730000, Peop. Rep. China
- SO Journal of Chemical Information and Computer Sciences (2003), 43(4), 1288-1296
 - CODEN: JCISD8; ISSN: 0095-2338
- PB American Chemical Society
- DT Journal
- LA English
- AB The support vector machine, as a novel type of learning machine, for the first time, was used to develop a QSAR model of 57 analogs of Et 2-[(3-methyl-2,5-dioxo(3-pyrrolinyl))amino]-4-(trifluoromethyl)pyrimidine-5-carboxylate (EPC), an inhibitor of AP-1 and NF-κB mediated gene expression, based on calculated quantum chemical parameters. The quantum chemical

parameters involved in the model are Kier and Hall index (order 3) (KHI3), Information content (order 0) (ICO), YZ Shadow (YZS) and Max partial charge for an N atom (MaxPCN), Min partial charge for an N atom (MinPCN). The mean relative error of the training set, the validation set, and the testing set is 1.35%, 1.52%, and 2.23%, resp., and the maximum relative error is less than 5.00%.

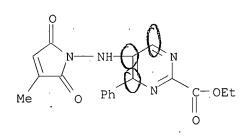
IT 561322-59-6

RL: PAC (Pharmacological activity); PRP (Properties); BIOL (Biological study)

(QSAR study of Et pyrimidinecarboxylates, inhibitor of AP-1 and NF-κB mediated gene expression based on support vector machines)

RN 561322-59-6 CAPLUS

CN 2-Pyrimidinecarboxylic acid, 5-[(2,5-dihydro-3-methyl-2,5-dioxo-1H-pyrrol-1-yl)amino]-4-phenyl-, ethyl ester (9CI) (CA INDEX NAME)



 \nearrow

Part Partisons are different both partisons

RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1994:534077 CAPLUS

DN 121:134077

TI Inverse Electron Demand Diels-Alder Reactions of Heterocyclic Azadienes: [4 + 2] Cycloaddition Reaction of Amidines with 1,3,5-Triazines

AU Boger, Dale L.; Kochanny, Monica J.

CS Department of Chemistry, Scripps Research Institute, La Jolla, CA, 92037, USA

SO Journal of Organic Chemistry (1994), 59(17), 4950-5 CODEN: JOCEAH; ISSN: 0022-3263

DT Journal

LA English

OS CASREACT 121:134077

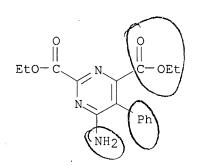
A detailed study of the scope of the amidine I (R = H, alkyl, etc.; $X \doteq$ AB NH2CH2CH2NH, etc.) Diels-Alder reaction with 1,3,5-triazines II (R = H, EtO2C, MeS) is described. The thermal reaction of amidines with sym. 1,3,5-triazines proceeds with in situ amidine to 1,1-diaminoethene tautomerization, [4+2] cycloaddn. with the 1,3,5-triazine, loss of ammonia from the initial Diels-Alder adduct with imine generation, imine to enamine tautomerization, and retro Diels-Alder loss of Et cyanoformate to provide substituted 4-aminopyrimidines in excellent conversions. reaction proceeds best with the amidine hydrochloride salts at intermediate reaction temps. (90-100 °C) in polar, aprotic solvents, is rather invariant to the ratio of dienophile-diene used (1:2 equivalent 1:1 equivalent. 2:1), and is subject to triazine substituent effects characteristic of an inverse electron demand Diels-Alder reaction (R = $CO2Et > R = H \gg R = SCH3)$. Notably, the generality of the amidine [4+2] cycloaddn. reaction with 1,3,5-triazines which was extended to include cyclic amidines effectively addresses the limitations of the alternative ynamine or N,O-ketene acetal dienophiles. A comparative examination of amidines, thioimidates, and imidates revealed that amidines are uniquely suited for use in this reaction cascade.

IT 157201-09-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 157201-09-7 CAPLUS

CN 2,4-Pyrimidinedicarboxylic acid, 6-amino-5-phenyl-, diethyl ester (9CI) (CA INDEX NAME)





- L4 ANSWER 8 OF 8 CAPLUS COPYRIGHT 2007 ACS on STN
- AN 1975:579010 CAPLUS
- DN 83:179010
- TI Competing cycloaddition in the reaction of 1,2,4-triazines with ynamines
- AU Reim, H.; Steigel, A.; Sauer, J.
- CS Inst. Chem., Univ. Regensburg, Regensburg, Fed. Rep. Ger.
- SO Tetrahedron Letters (1975), (33), 2901-4 CODEN: TELEAY; ISSN: 0040-4039
- DT Journal
- LA German
- OS CASREACT 83:179010
- The triazines I (R = H, Ph, R1 = H) with MeC.tplbond.CNEt2 gave 100% pyrimidines II by 2,5-addition I (R = H, R1 = Ph), for which 2,5-addition is blocked by Ph, gave 85% pyridine III (R2 = Me, R3 = NEt2) as the only product by 3,6-addition I (R = R1 = CO2Me, Me) gave mixts. of II and III (R2 = Me, R3 = NEt2) and similarly, with PhC.tplbond.CH, gave III (R2 = Ph, R3 = H; R2 = H, R3 = Ph). I (R = R1 = Ph) with MeC.tplbond.CNEt2 gave II and III (R2 = Me, R3 = NEt2; R2 = NEt2, R3 = Me) similar reactions with MeC.tplbond.CNMe2 gave analogous results. The proportions of the mixts. obtained were solvent dependent.
- IT 57767-98-3P 57768-01-1P
 - RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)
- RN 57767-98-3 CAPLUS
- CN 2-Pyrimidinecarboxylic acid, 4-(diethylamino)-5-methyl-6-phenyl-, methyl ester (9CI) (CA INDEX NAME)

- RN 57768-01-1 CAPLUS
- CN 2-Pyrimidinecarboxylic acid, 4-(dimethylamino)-5-methyl-6-phenyl-, methyl ester (9CI) (CA INDEX NAME)

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(FILE 'HOME' ENTERED AT 23:01:59 ON 02 AUG 2007)

FILE 'REGISTRY' ENTERED AT 23:02:09 ON 02 AUG 2007

L1 STRUCTURE UPLOADED

L2 3 S L1 SSS SAM

L3 69 S L1 SSS FUL

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L4 8 S L3

FILE 'CAOLD' ENTERED AT 23:04:07 ON 02 AUG 2007

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COST IN U.S. DOLLARS SINCE FILE TOTAL ENTRY SESSION

FULL ESTIMATED COST 0.45 215.84

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS) SINCE FILE TOTAL

CA SUBSCRIBER PRICE ENTRY SESSION 0.00 -6.24

STN INTERNATIONAL LOGOFF AT 23:04:20 ON 02 AUG 2007